Mesocale approach for fluidized beds

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1 Introduction

Fluid-particle flows are frequently encountered in industrial facilities and especially in chemical engineering processes. In this work, we focus on fluidized beds, which involve a fluid flow passing upward through a pack of particles with such a velocity that the fluid force acting on particles is larger than their weight. This technology is commonly used for its high heat and mass transfer rates in Circulating Fluidized Beds or Fluid Catalytic Cracking processes which are composed of millions of particles from a few micrometers to some millimeters, fluidized by a liquid or a gas. In order to optimize performances of those engineering processes, numerical simulations of multiphase flows became indispensable, especially over the last 20 years with the considerable rise of computational power and the progress in multiphase computational fluid dynamics. Depending on the length scale, there are three main approaches to simulate the dense particulate flows in fluidized beds (see fig 1).

At the micro-scale, the fluid motion equations are solved directly on a small mesh compared to the particle diameter. Direct numerical simulation (DNS) provides precise solutions but the number of fluid cells does not permit to simulate systems containing more than a few thousands particles in a reasonable computing time.

At the macro-scale, by using Eulerian methods, the fluid and solid phases are considered as two inter-penetrating media. The mesh is then coarser than a particle diameter and simulation of large domains, up the real size reactor, are doable. However, this length scale requires the introduction of numerous assumptions in the model to describe the evolution of the solid phase and its coupling with the surrounding fluid. Moreover, since the solid phase is considered as a continuous media, particle trajectories are not individually treated, which is a crucial lack of information for engineering processes.

At an intermediate scale between the DNS and Euler-Euler methods, the fluid is solved on a larger grid than the particle diameter, as it is in the Euler-Euler methods, but as in DNS methods, the particle trajectories, including collisions, are tracked with a discrete element method (DEM). This approach, commonly called discrete element method / computationnal fluid dynamics (DEM-CFD) or Euler-Lagrange method, was first introduced by Tsuji *et al.* [7] and Hoomans *et al.* [5]. This method has been widely developped and used since the beginning of the XXIst century (see *e.g.* [6, 11]).

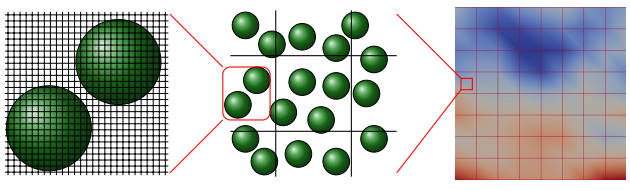


Figure 1: Different length scales used for simulating fluid-particle flows

2 Model equations and numerical techniques

2.1 Particle trajectories

The translational and rotational motion of a particle i with mass m_i is calculated using Newton's second law of motion :

$$m_i \frac{d\mathbf{v}_i}{dt} = \mathbf{f}_{g,i} + \mathbf{f}_{pp,i} + \mathbf{f}_{fp,i} \tag{1}$$

Where $\mathbf{v}_p$ and ω_p are the translational and rotational velocities, respectively. $\mathbf{f}_g$, $\mathbf{f}_{pp}$ and $\mathbf{f}_{fp}$ are the gravity force, the contact force and the hydrodynamic force eperienced by the particles embedded in the fluid respectively (see subsection 2.3).

The collision model used in this work is based on a soft-sphere / discrete element model, allowing colliding particles to slightly overlap to compute the contact forces. Contact forces considered here are a normal elastic restoring force, a normal viscous dynamic force and a tangential friction force. Particle trajectories and contacts are solved with the IFPEN granular code GRAINS3D [10].

2.2 Fluid motion

The fluid motion is described with spatially averaged continuity and momentum balance equations introduced by Anderson and Jackson [2]. In this work, the B model (see [4]) formulation of the two fluid model (TFM) is used :

$$\begin{cases} \dfrac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon \mathbf{u}_f) = 0, & \text{(2a)} \\ \dfrac{\partial (\rho_f \varepsilon \mathbf{u}_f)}{\partial t} + \nabla \cdot (\rho_f \varepsilon \mathbf{u}_f \otimes \mathbf{u}_f) = -\nabla P + \mathbf{F}_{pf} + \nabla \cdot (\varepsilon \tau) + \varepsilon \rho_f \mathbf{g} & \text{(2b)} \end{cases}$$

Where $\mathbf{u}_f$, ρ_f, P and τ are the fluid velocity, density, pressure and stress, respectively. $\mathbf{F}_{pf}$ is a volumetric force modelling the particle-fluid interaction. The fluid volume fraction ε is calculated with respect to the number of particles in each fluid cell.

Navier-Stokes equations (2) are solved using a Marchuk-Yanenko first order operator splitting for time integration. For the space discretization, a classical finite volume / staggered grid scheme is employed.

2.3 Two-way coupling

In order to respect Newton's third law of motion, the volumetric particles-on-fluid force, $\mathbf{F}_{pf}$, must balance the sum of fluid-on-particle forces, $\mathbf{f}_{fp}$, in each cell :

$$\mathbf{F}_{pf} = -\frac{\sum_{i=1}^{n_c} \mathbf{f}_{fp,i}}{\Delta V} \tag{3}$$

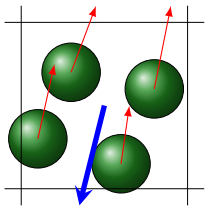


Figure 2: Interaction forces

The fluid-on-particle force is obtained by integrating the total fluid stress on the boundary of each particle. Considering the local averaging process introduced by Anderson & Jackson [2], the fluid stress σ can be decomposed into its local mean value $\overline{\sigma}$ and a fluctuation term σ'. As $\sigma = -P\ \delta_{ij} + \tau_f$, fluid-on-particle force can be expressed as the sum of a hydrostatic contribution and a hydrodynamic contribution. In this work, only drag and buoyancy forces are considered, hence the fluid-on-particle force reduces to :

$$\mathbf{f}_{fp} = -V_p \rho_f \mathbf{g} + \mathbf{f}_d \tag{4}$$

We employ the drag force correlation suggested by Di Felice [3], which shows good predictions over a large range of particle concentration and Reynolds number.

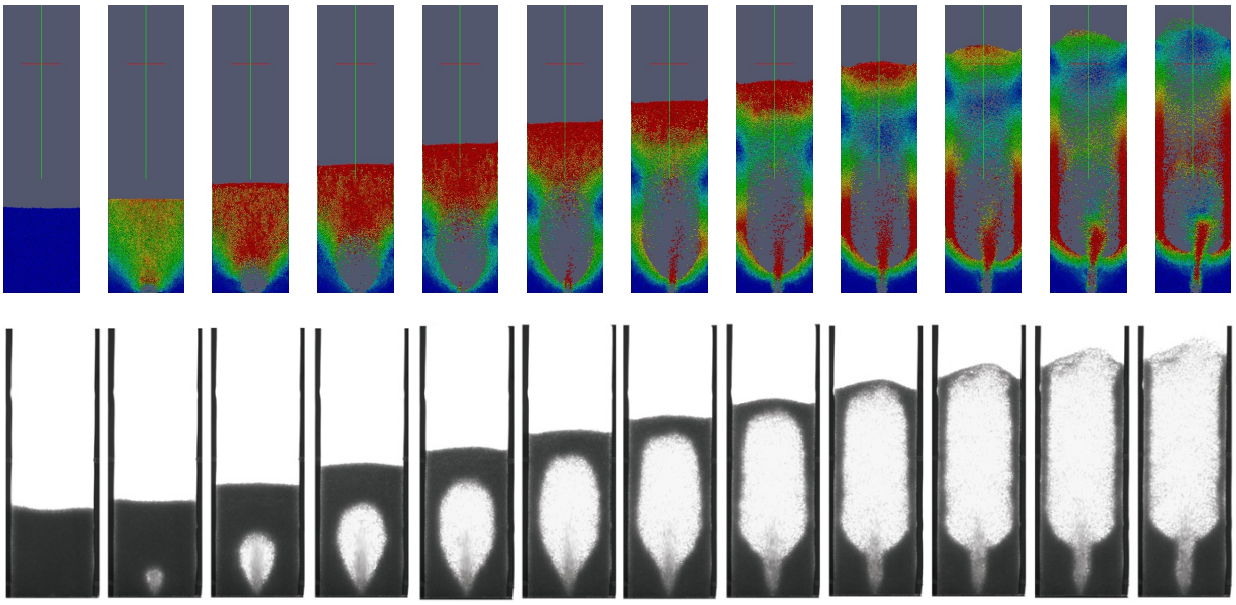


Figure 3: Comparison between PeliGRIFF simulation and experimental data of Alobaid *et al.* [1]

3 Validation tests

The DEM-CFD model presented in section 2 has been implemented in the IFPEN PeliGRIFF platform [8, 9]. Several validation tests have been performed, both in bubbling and spouting regimes as illustrated in figure 3.

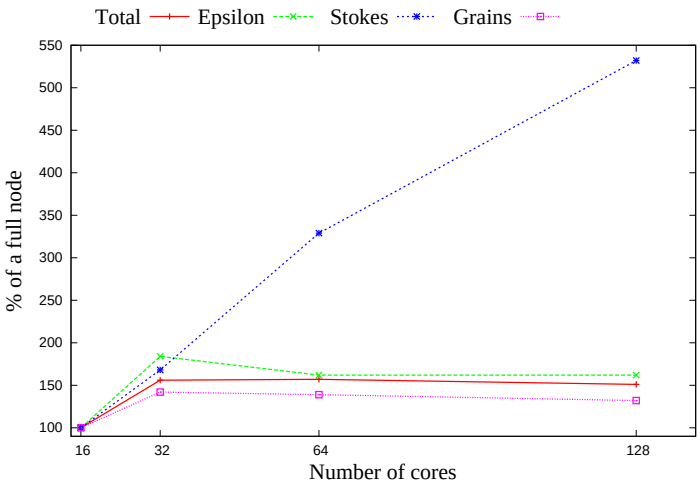
The C++ code PeliGRIFF is fully MPI using non blocking communication pattern and data exchange between fluid and granular solvers has been optimized. Figure 4-a shows the evolution of the computing time in the different parts of the code with respect to the number of computing cores. Computing time is normalized by a full node (*i.e.* 16 cores) computing time.

The particles and fluid cells load per core is constant in our test, thus we expect that the computing time is constant on 32, 64 and 128 cores for a twice, 4 times and 8 times larger problem than the 16 cores one. The Stokes problem solution does not scale very well due to the low fluid cells load per core but it represents only a few percents of the total computing time (see table 4-b). However, the rest of the code scales very well beyond 2 full nodes and the global parallel behaviour of the implementation is deemed to be satisfactory.

30000 and 120000 particles per core simulations have be performed on up to 128 cores, *i.e.* up to 15 millions of particles, with the same good parallel behaviour. That opens the way to simulations of several hundred millions of particles on a larger number of cores, which is close to some engineering processes size.

4 Ongoing work

The multi-scale framework we wish to build implies to transfer information from DNS at the micro-scale to the DEM-CFD model at the meso-scale. To achieve this goal, we are currently investigating the same system (a fluidized bed containing a few tens of thousands of particles) both by DNS and DEM-CFD simulations. Simultaneously, additional DEM-CFD simulations are performed to examine the particles kinetic energy and collision rate evolution with respect to time, inlet velocity and bed height.



(a)

	Node(s)			
Part	1	2	4	8
Stokes	1%	2%	3%	4%
Epsilon	12%	15%	15%	14%
Grains	81%	80%	84%	78%

(b)

Figure 4: Scale-up results with constant load per core (30000 particles). (a) Time repartition evolution, (b) Time repartition in percents.

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